LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

UCRL-TR-224286

The Computation Directorate at Lawrence Livermore National Laboratory

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Updated October 14, 2003

The Computation Directorate
At Lawrence Livermore National Laboratory

May 2006

Computation Directorate
Lawrence Livermore National Laboratory

Outline

- Overview of the Laboratory
- Overview of the Computation Directorate
- Facilities
- Livermore Computer Center
- LLNL and Computation Support for Important National Missions

LLNL is managed by the University of California for the NNSA

Our Mission:
National Security
in a Global Context

- Multi-program
- Multi-disciplinary
- "Big Science"

- $1.6B annual budget
- 8300 employees
- 1 square-mile main site
- Experimental test site

- National Security
- Homeland Security
- Energy & Environment
- Applied Science

Computation Directorate Vision and Mission

Vision

Computation aspires to be the preeminent high performance computing and computer science organization in order to enable scientific discovery and Laboratory missions.

Mission

Computation assures Laboratory mission and program goals are attained by delivering outstanding computer science expertise, world-class high performance computing capabilities, and creative technology and software solutions.

Work in Computation

- **The Computation Directorate has <u>four major areas</u> of work:**
  - **Programmatic Support:**
    - Programs are areas which receive funding to develop solutions to problems or advance basic science in their areas.
      - Ex: Stockpile Stewardship, Homeland Security and the Human Genome project
    - Computer scientists are “matrixed” to these programs to provide computer science support
  - **Livermore Computer Center (LCC):**
    - Development, support and advanced planning for the large, massively parallel computers, networks and storage facilities used throughout the laboratory
  - **Research:**
    - Computer scientists research advanced solutions for programmatic work and for external contracts and research new HPC hardware solutions
  - **Infrastructure:**
    - Support for thousands of desktop computers and numerous LANs, lab-wide unclassified networks, computer security, computer-use policy.

LLNL Computer Facilities and Infrastructure

New Terascale Simulation Facility houses ASC Purple and BG/L supercomputers

LLNL now has the most capable computing infrastructure in DOE

- State-of-the-art facility in the center of the Lab
- Two unobstructed computer floors totaling > 1 acre (almost a football field of computer space!)
- Total power 12MW to power and cool computers (up to 15MW)
- 280 offices, meeting rooms, visualization theaters, operations support, tape vault, labs

LLNL
Exploration in petascale computing

Vendor-integrated MPP
production stability

100TF ASC Purple

1,536 nodes
12,288 Power5 processors
50 TB memory
AIX software

Linux clusters
cost-effective science

23TF Thunder Linux cluster

1,024 nodes
4,096 processors
16 TB memory
Linux software

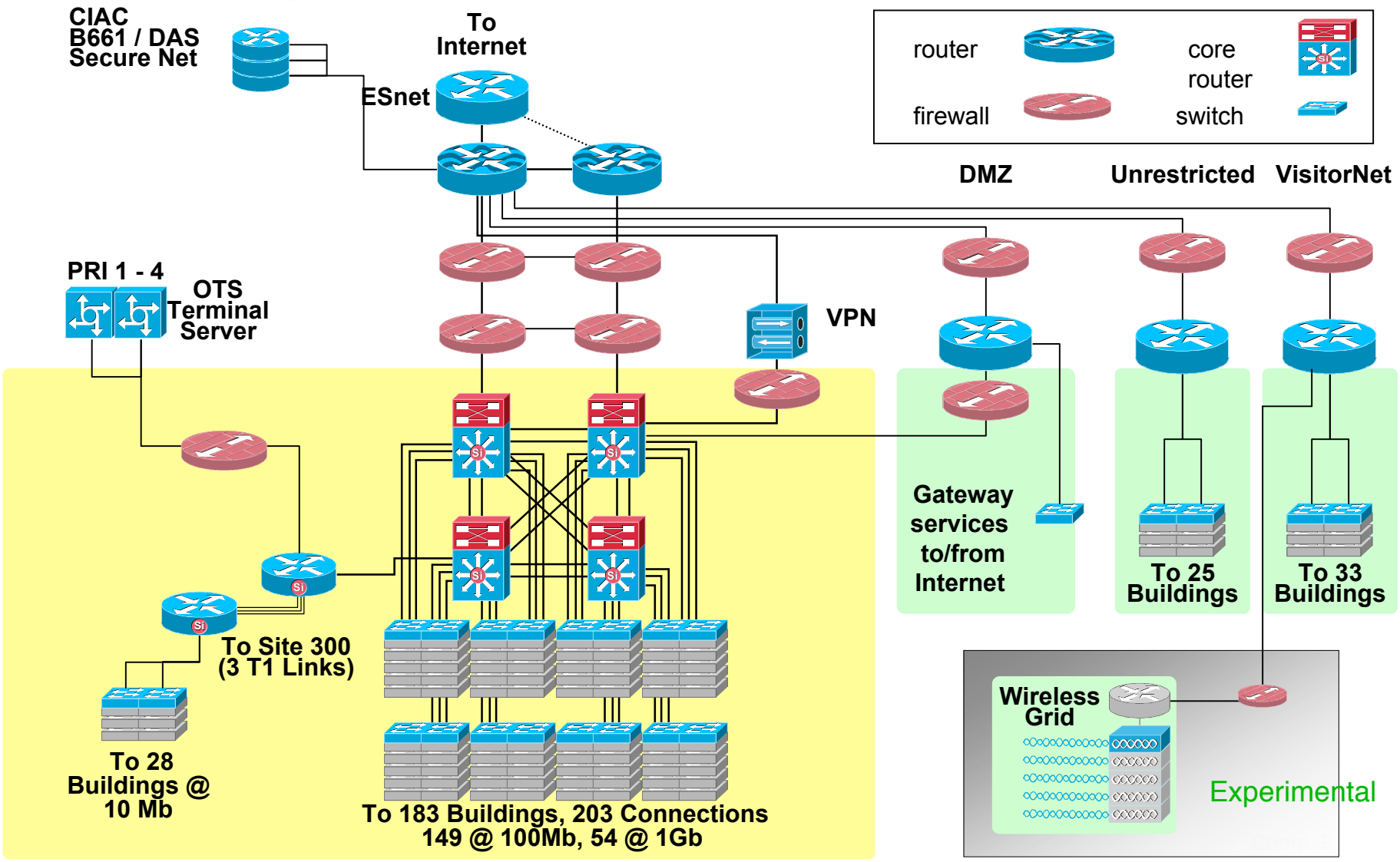
Novel architectures
leading edge

360TF BlueGene/L

65,536 nodes
131,072 processors
32 TB memory
64 cabinets
1.5 MW
2500 square feet

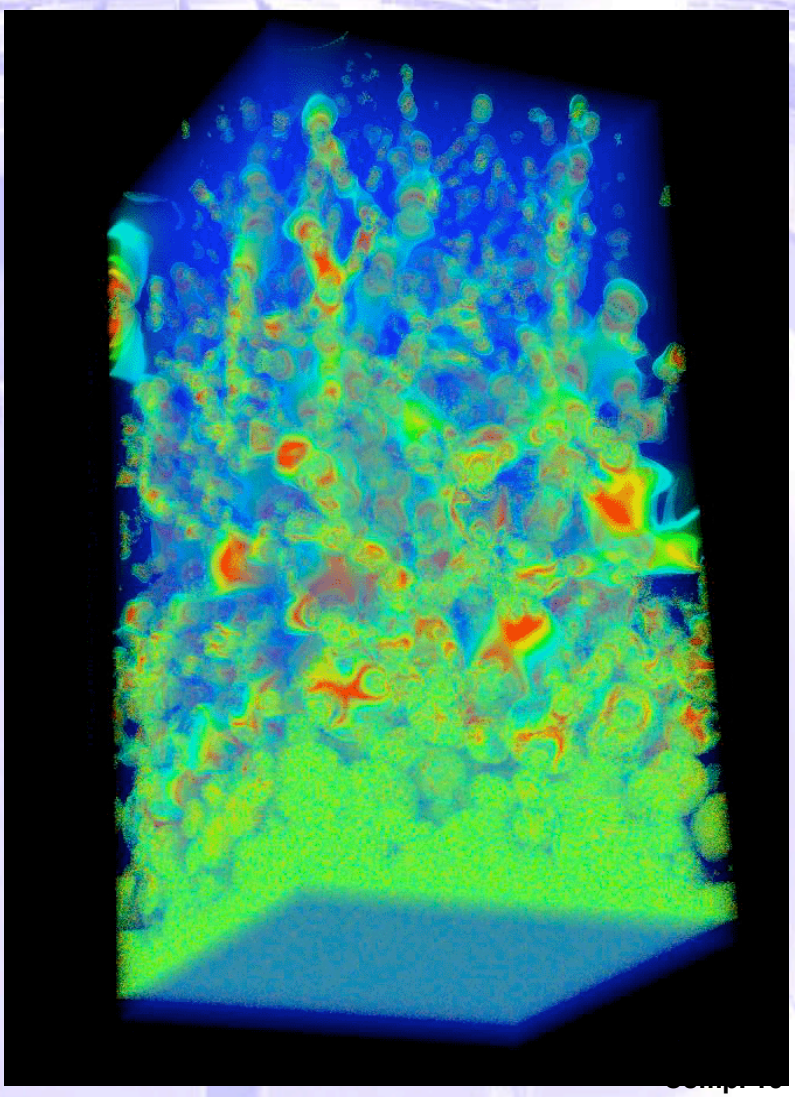
BlueGene/L is the world's fastest supercomputer at 360TF and Purple is #3 on the Top500 list of the world's fastest supercomputers!!

Big Computers – Powerful Networks



Central Computer Services / Support

- Customer Support, Hotline, Technical Consulting, Account Management
  - Online Documentation, HPC Training & Education, Customer Outreach
- Software and tools development for High Performance Computing (HPC) User support:
  - Compilers
  - Memory tools
  - Debuggers
  - Performance analysis tools
  - Software evaluation
  - In-depth consulting
  - Tools development
  - Vendor collaborations
  - And more…
- Development and support of tools for managing, visualizing and presenting scientific data.



Central Computer Services / Support

- **Network Services**
  - **Email**
    - Anti-Spam
    - Anti-Virus for email
    - Mailing lists (majordomo)
    - Pop Servers
  - **Calendaring (Meeting Maker)**

- **System Support Services**
  - **Active Directory**
  - **Imaging**
  - **Software Distribution**
  - **Configuration inventory**
  - **OS Patch Management**
  - **Desktop Anti-virus**

- **Computation Training Center**

- **4Help Central help desk**
  - **Desktop application support**
  - **Network, desktop and computer security services support**
  - **Remedy trouble ticket system**

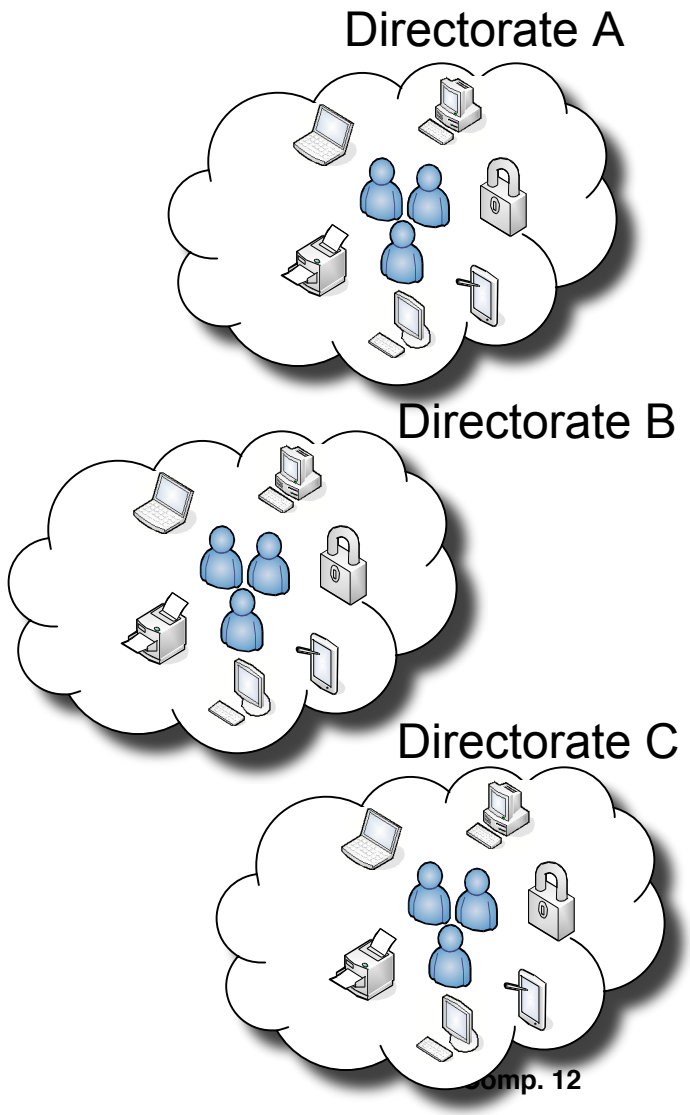
Content filtering

Anti-spam

Anti-virus

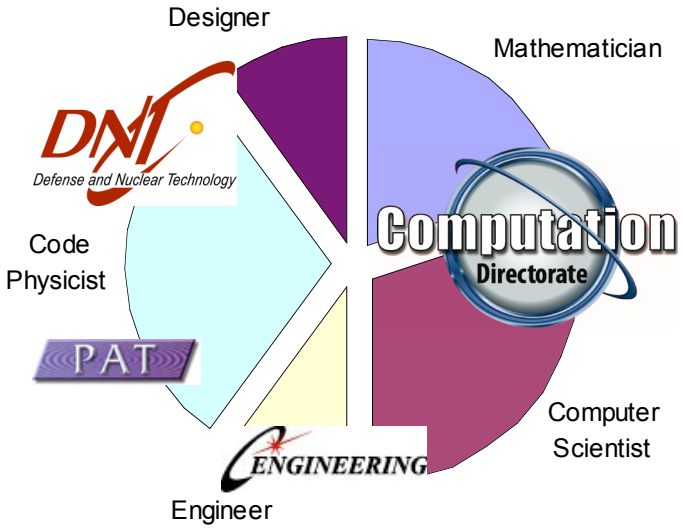
LAN, Network and Desktop Support

- A large staff of System Administrators provides IT Support for LLNL Directorates
  - Hardware Support
  - OS Support
  - Software installation and troubleshooting
  - Network Support
  - Computer Security
  - IT Project Management



Overview of LLNL's Programs and Computer Science Support for these Programs

A Code Team at LLNL



A typical project or code team draws expertise from several disciplines. A team developing a physics simulation code would include physicists, computer scientists, mechanical engineers, mathematicians and possibly a chemist.

Nonproliferation / Homeland Security

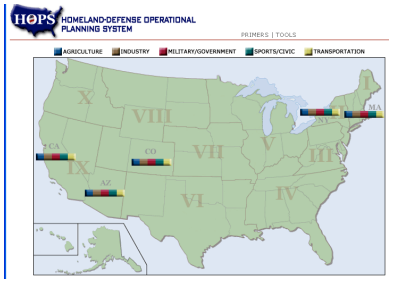
LLNL is a premier developer of systems solutions to preclude the proliferation, acquisition, or use of weapons of mass destruction.

This includes work in terrorism prevention, proliferation detection, incident response, international assessment of WMD capabilities.

Nonproliferation / Homeland Security

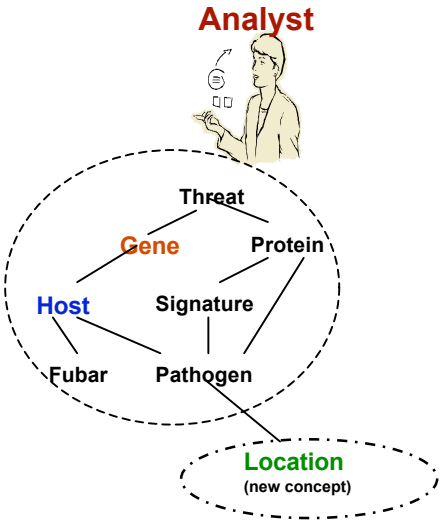
Computer scientists develop conflict simulation codes, map and analyze networks for vulnerabilities, develop graph search tools, and develop text analysis and data fusion technology.

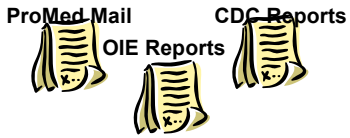
Joint Conflict & Tactical Simulation



Homeland Defense Operational Planning System (HOPS)

Text analysis

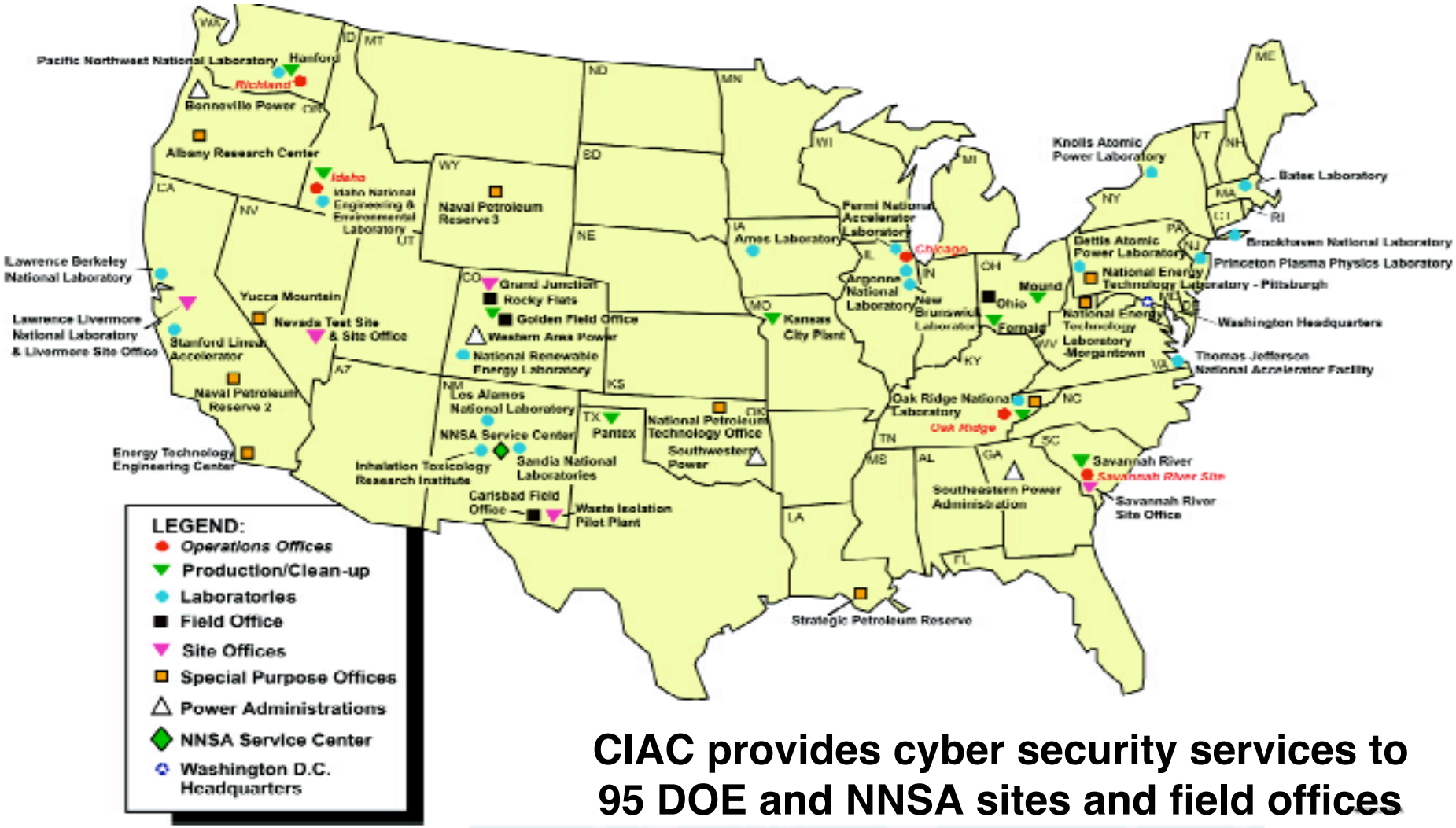




Entity and event extraction

Classification and clustering

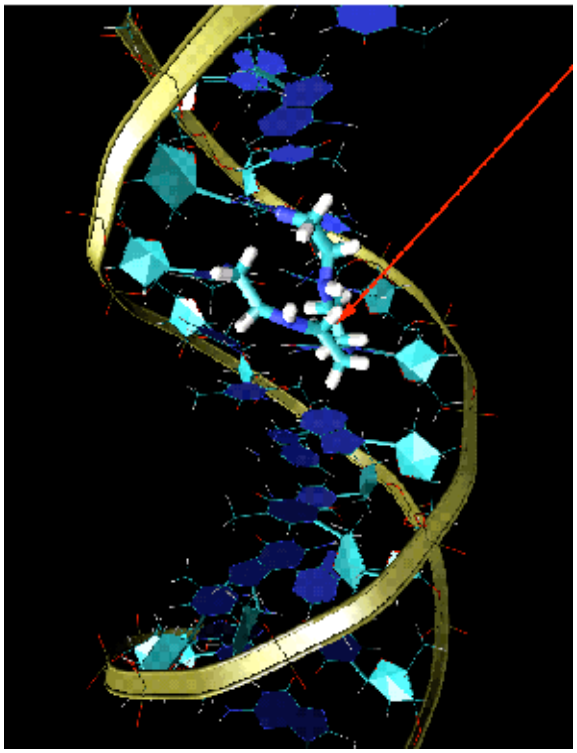
Nonproliferation / Homeland Security - Computer Incidence Advisory Capability



CIAC provides cyber security services to 95 DOE and NNSA sites and field offices

Biosciences

Bioscience research at LLNL is a program in molecular biology, genetics, genomics, computational biology, and biotechnology. These efforts are in the service of three main areas of societal need: human health, defense biology, and environmental health.



Computer Scientists develop genomic databases, web tools to access this data and data mining tools.

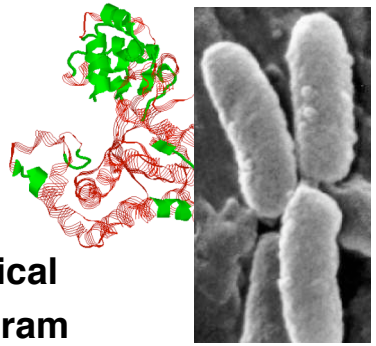
Skills: Bioinformatics, Java, web technology, some Perl and C

Biosciences – cont.

Computer Scientists at LLNL were the first to develop software to identify pathogins. This work supports DHS bio-science and bio-security goals

In 20 minutes, KPATH identified a unique region of the SARS genome, leading the way for human diagnostics

LLNL has earned a lead role within DHS for pathogen informatics

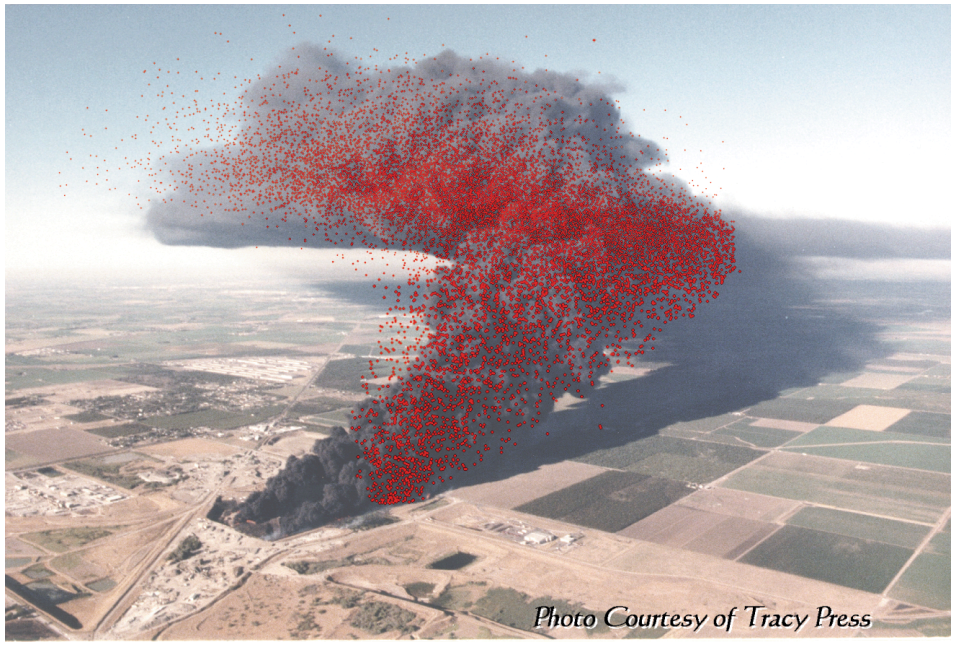


Chemical and Biological Nonproliferation Program

Atmospheric and Climate Modeling

LLNL develops codes to do climate, ocean and atmospheric modeling. The example to the right is a simulation superimposed on a real picture of a tire fire in Tracy, CA.

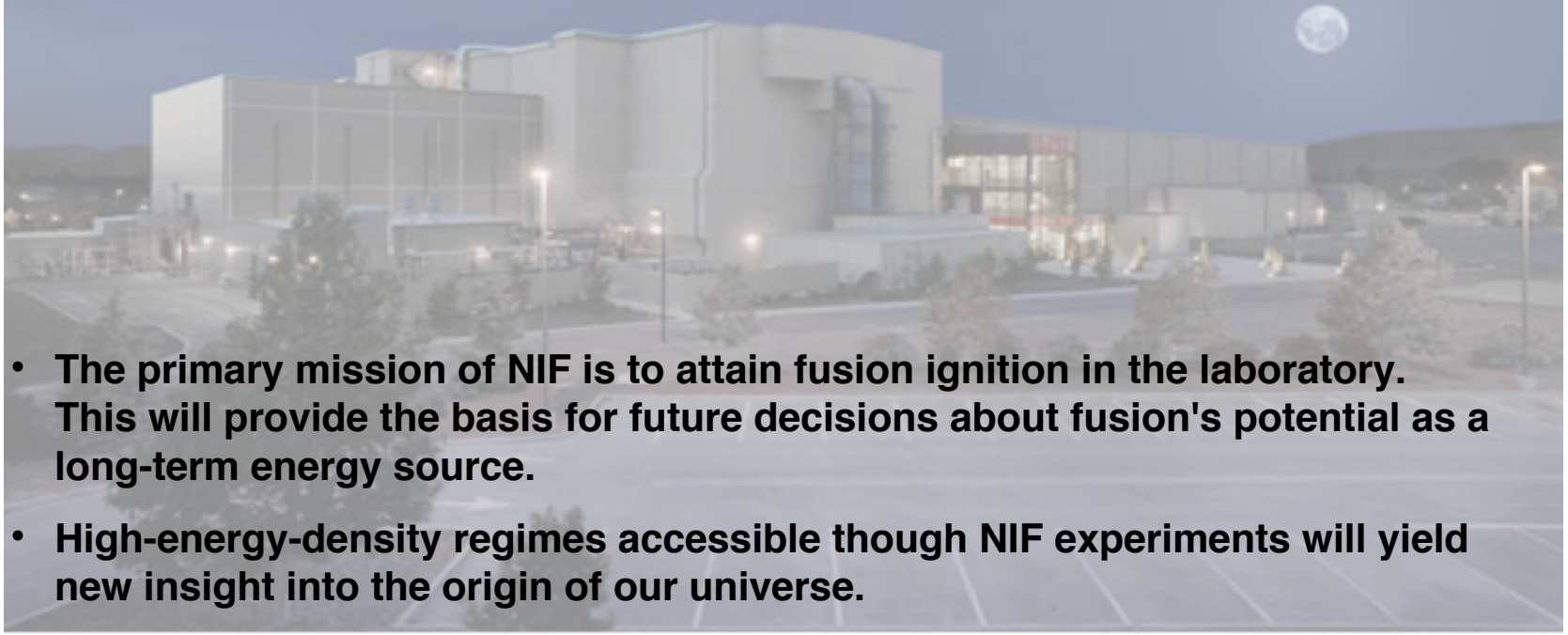
The National Atmospheric Release Advisory Center uses this predictive capability to map the probable spread of hazardous materials released into the atmosphere such as during the Chernobyl disaster.



Computer Scientists work with other scientists to develop these atmospheric, ocean and climate modeling codes and supporting tools.

The National Ignition Facility (NIF)

- NIF is a key component of the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program, whose mission is to maintain the safety, reliability, and effectiveness of our nation's nuclear stockpile without underground nuclear testing.



- The primary mission of NIF is to attain fusion ignition in the laboratory. This will provide the basis for future decisions about fusion's potential as a long-term energy source.
- High-energy-density regimes accessible though NIF experiments will yield new insight into the origin of our universe.

National Ignition Facility at night

NIF

Computer Scientists team with Engineers to develop control system software such as shown to the left. They also develop database applications, and analysis software in support of NIF.

Skills: OO, embedded systems, Oracle, Java and user interface design

Stockpile Stewardship

Stewardship of the U. S. nuclear stockpile is the foremost responsibility of the Lawrence Livermore National Laboratory. In the absence of nuclear testing, we now rely on interrelated computer calculations, validated by non-nuclear experimental results and benchmarked against past nuclear test data, for the continued certification of the stockpile.

Stockpile Stewardship – cont.

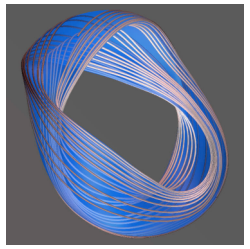
Eric is the Project Leader for the VisIt visualization code that is displaying the data to the left. In 2005, Eric and his team won an R&D 100 Award.

Here VisIt is being used to show the density analysis of a National Ignition Facility test target under laser bombardment.

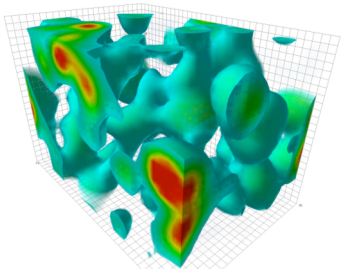
Computer Scientists work with Physicists to develop the simulation codes that support the Stockpile Stewardship program. They also develop the support tools such as the parallel visualization codes to display this data.

CASC
Center for Applied Scientific Computing

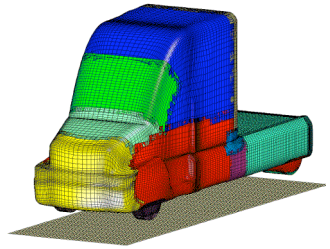
CASC basic math research tackles difficult simulation science needs



- **Scalable linear solvers**
  - **Fundamental algorithm research in optimal-complexity multigrid methods**
  - **Massively parallel implementations**



- **PDEs in complex geometry**
  - **Fundamental research in efficient meshing and discretization methods**



- **Multiscale Mathematics**
  - **Improved kinetic algorithms for moderately collisional plasmas**

Software Quality Assurance

LLNL Software Quality Assurance initiative

- **Institutionally-funded SQA program provides framework for quality and compliance**

- **Our Computer Scientists are a resource within LLNL and across DOE**
  - **LLNL chairs DOE SQA Subcommittee**
  - **LLNL Computer Scientists participate on DOE safety software assessments**
  - **LLNL programs requesting SQA consulting and assessments**

Institute for Scientific Computing Research – Academic Connections

Summer Program

91 students and
11 faculty

Seminars & Visitors

252 visits and
84 seminars

Lasting Relationships

Sabbatical visitors
Students & postdocs
Workshops & conferences

Extensive interactions with UC

UCSD (data sciences)

UCD (visualization)

UCLA (IPAM affiliate)

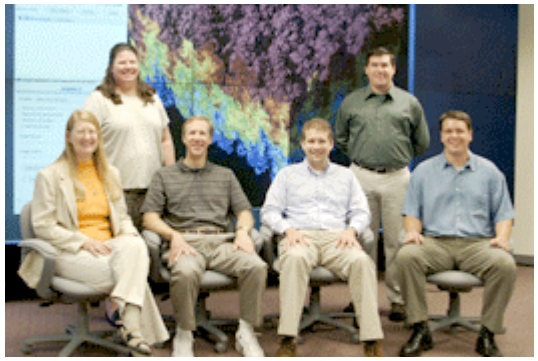
PI-to-PI interactions at 9 campuses

Computer Scientists recognized for significant contributions

Two R&D 100 Awards

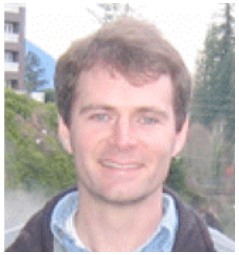
Eric Brugger, Sean Ahern, Kathleen Bonnell, Hank Childs, Linnea Cook, Jeremy Meredith, Mark Miller, Brad Whitlock, *VisIt software*

David Pletcher, Jim Schek, *Adaptable Radiation Area Monitor*



Sapphire Team earns three more patents

Chandrika Kamath and her team earned three more patents for their work in scientific data mining



Featured publications

Ivan Ovcharenko's article on Gene Deserts and Regulatory Elements is featured on cover of *Genome Research*

Michael Wickett contributes to climate studies deemed one of Top 100 science stories of 2005 by *Discover Magazine*

CAR scientists on 3 of 6 Gordon Bell Prize finalists

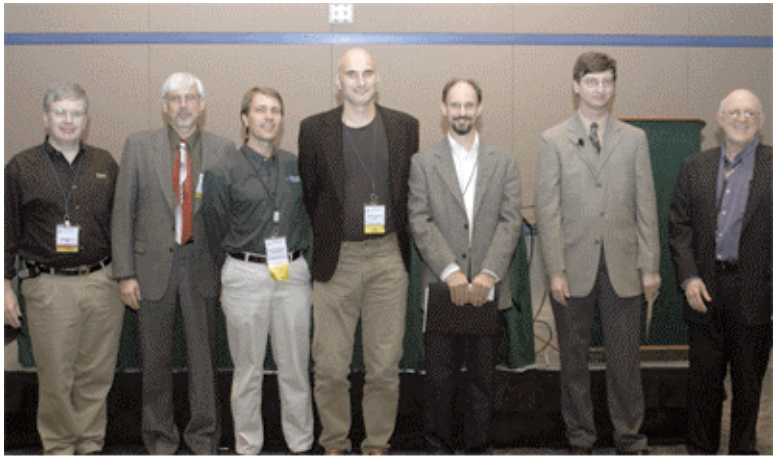
Erik Draeger, Bor Chan, Keith Henderson, Bronis de Supinski, Kim Yates, Andy Yoo

Computer Scientists on three of six Gordon Bell Prize finalists

Gordon Bell Prize Winner

100+ TFlop Solidification Simulations

- **Fred Streitz (PAT), Kim Yates, Bronis de Supinski, Bor Chan with colleagues from IBM**



The Gordon Bell award-winning team (from left): James Sexton of IBM, Kim Yates, Bronis de Supinski, James Glosli, and Fred Streitz of LLNL, are pictured with Bill Gropp of Argonne, who chaired the prize committee, and C. Gordon Bell. Team members not pictured are Mehul Patel and Bor Chan from LLNL, and John Gunnels of IBM.

Two other finalists

Large-Scale FMPD Simulations

- **Francois Gygi, Erik Draeger, Bronis de Supinski, Kim Yates with colleagues from Carnegie-Mellon, Vienna University of Technology, and IBM Watson**

Scalable Breadth-First Search Algorithm

- **Andy Yoo, Keith Henderson with colleagues from Sandia, Ohio State, and D.E.Shaw**

BlueGene/L and Purple are the #1 and #3 fastest computers in the world

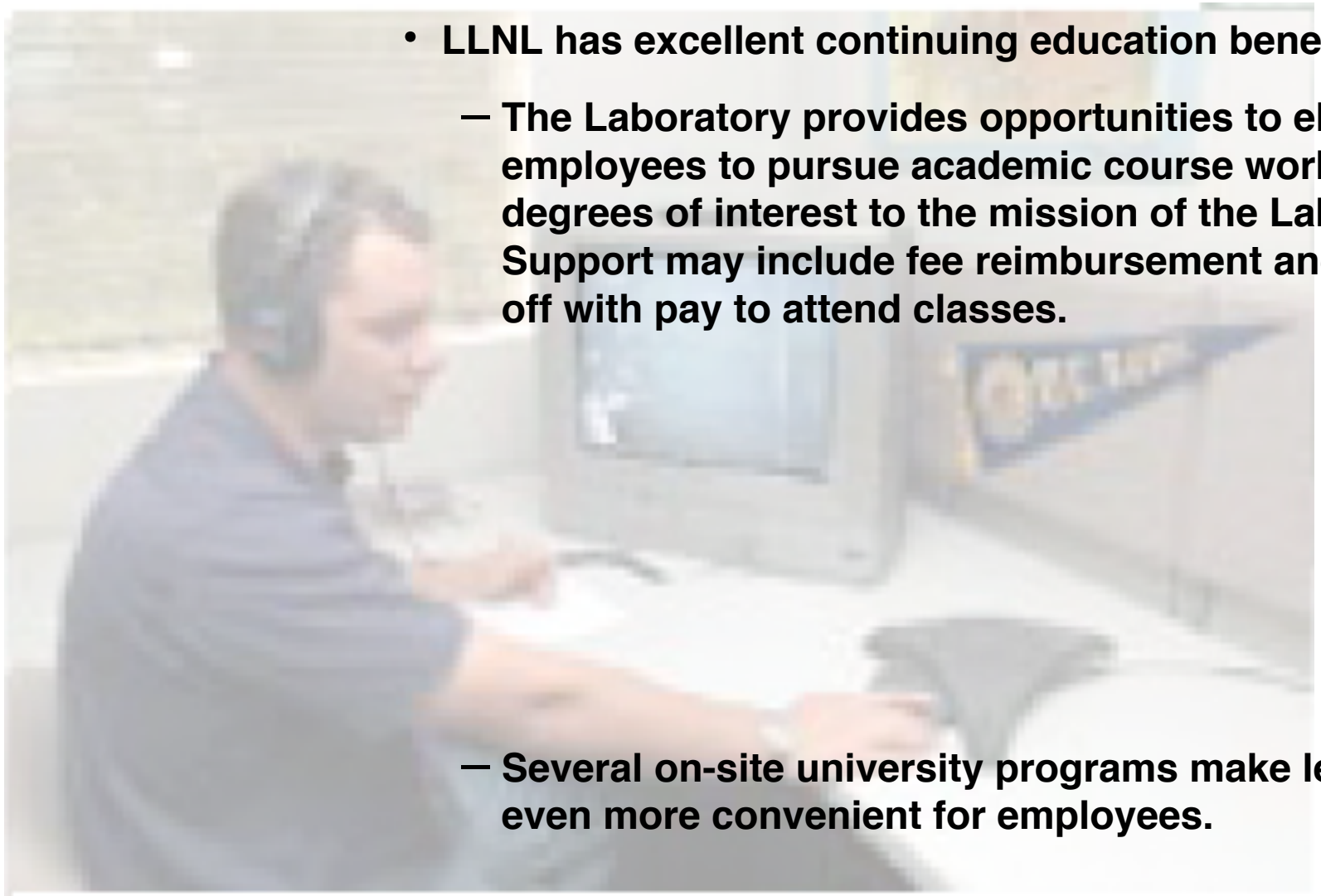
- **Blue Gene/L #1 (280.6 teraflops on Linpack)**
- **Purple #3 (63.39 teraflops on Linpack)**

Accepting award, Dr. Dimitri Kusnezov, Director of NNSA ASC

Accepting award Tom Spelce, LLNL and Dr. Tilak K. Agerwala, IBM T. J. Watson Research Center

Blue Gene/L swept all four HPC Challenge Class 1 benchmark awards

Continuing Education



- LLNL has excellent continuing education benefits
  - The Laboratory provides opportunities to eligible employees to pursue academic course work and degrees of interest to the mission of the Laboratory. Support may include fee reimbursement and/or time off with pay to attend classes.
  - Several on-site university programs make learning even more convenient for employees.

Disclaimer and Auspices

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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